One-dimesional crystals and heat superconductivity

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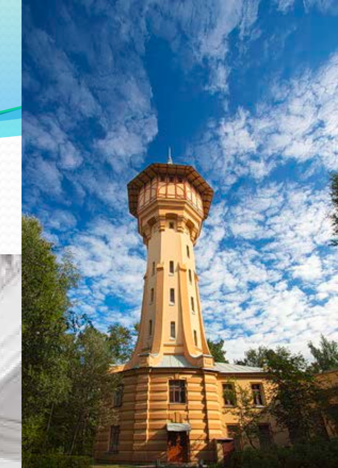
43 International School-conference

The first Summer School was organized by **Ya. G. Panovko** and his colleagues in **1971**

Peter the Great St. Petersburg Polytechnic University



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  - M.V. Simonov
  - D.V. Tsvetkov

Maxwell's demon

It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of nonconducting crystals.

Rudolf Peierls

Breakdown of Fourier's law in perfect low-dimensional systems

$$\mathbf{h} = -\kappa \nabla T$$

Heat flux

Heat conductivity

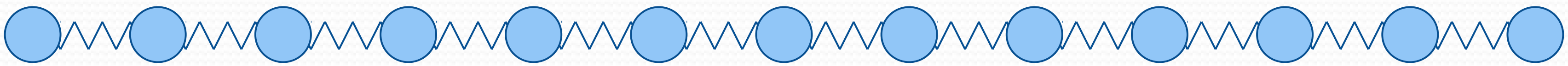
Temperature

Review papers:

Heat transport in low-dimensional systems
A. Dhar, Advances in Physics, 57 (5), **2008**.

Fourier's law: A challenge for theorists
Bonetto, Rey-Bellet, Lebowitz, **2000**
In Mathematical physics, Imperial college press, London

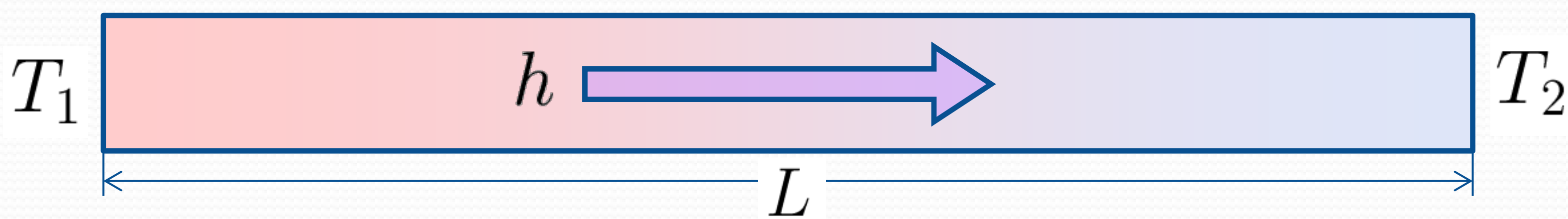
Theory: breakdown of Fourier's law in perfect low-dimensional systems



Properties of a harmonic crystal
in a stationary nonequilibrium state
Rieder, Z., **Lebowitz**, J.L., Lieb, E.
Journal of Mathematical Physics
Vol. 8, Iss. 5, **1967**, P. 1073-1078

Fourier's low:

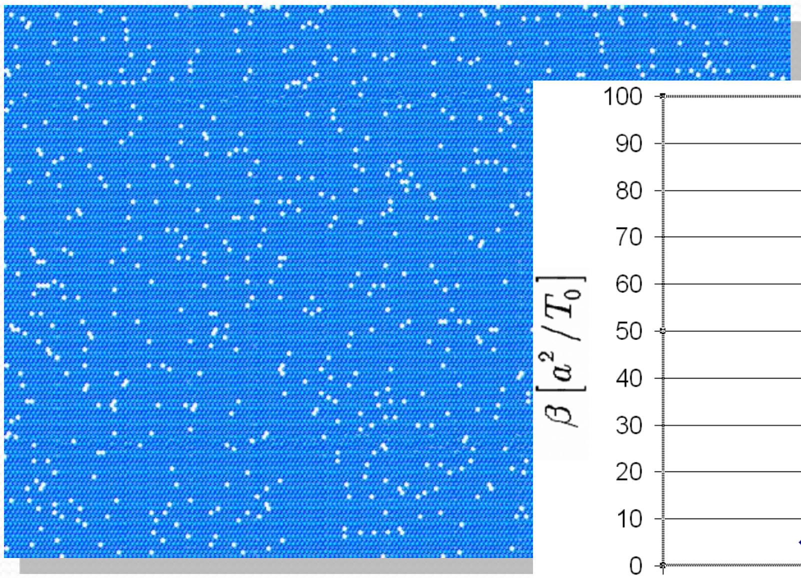
$$h = -\kappa T' \approx \kappa \frac{T_1 - T_2}{x_2 - x_1}$$

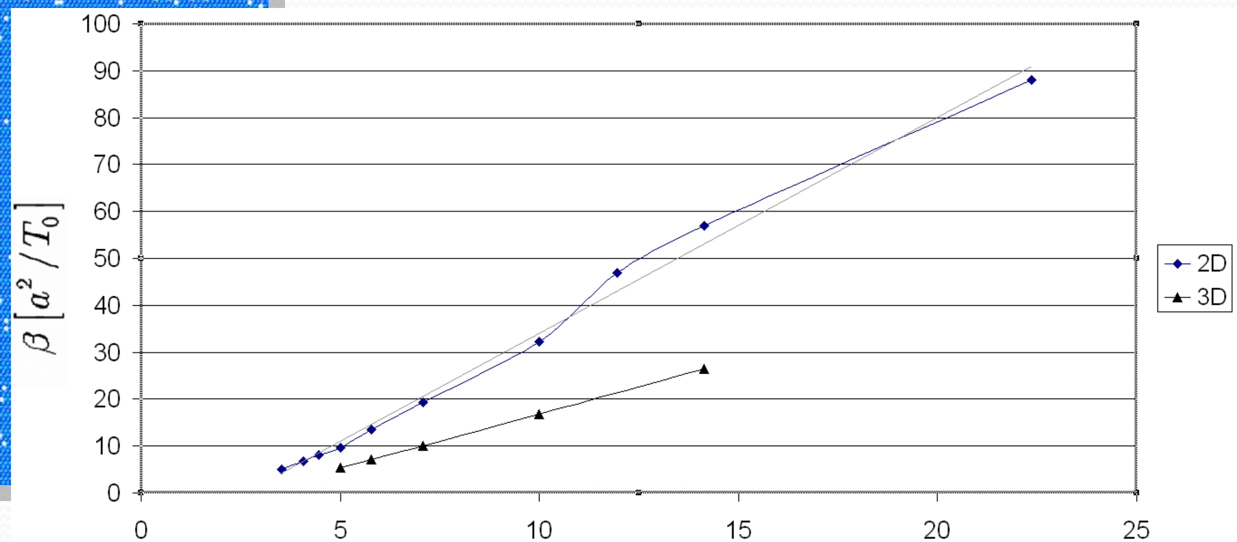


$$1D: \qquad h \sim T_1 - T_2, \qquad \kappa = \frac{L}{T_1 - T_2} h \sim L$$

Heat superconductivity

Fourier's law fulfills for perfect crystals with randomly distributed vacancies





- Heat conductivity is proportional to inverse square root of defect density

$$\kappa \sim \rho^{-1/2}$$

A.A. Le-Zakharov, A.M. Krivtsov, Doklady Physics, 2008

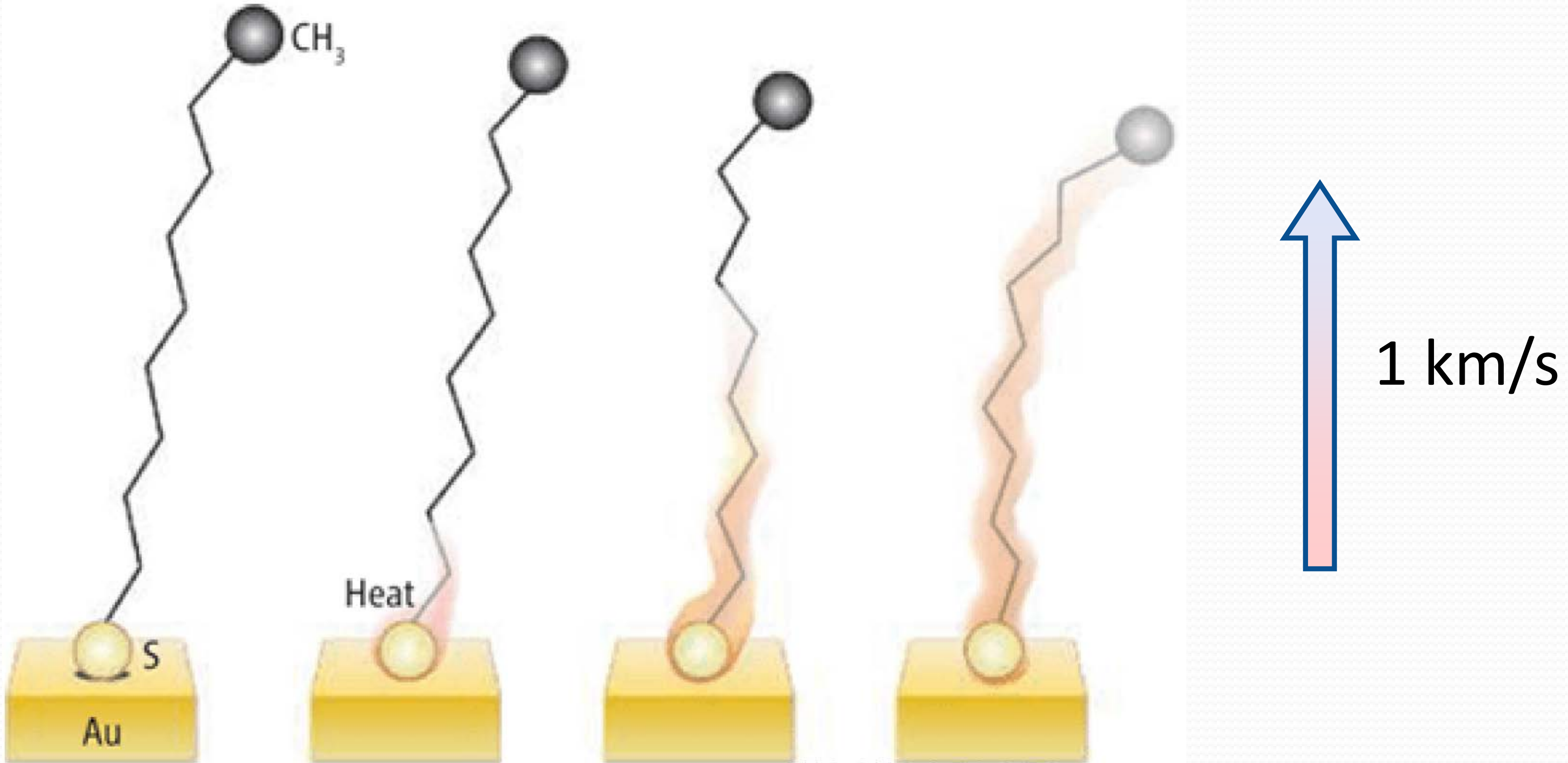
Heat superconductance: experimental confirmation

Science 10 August 2007
Vol. 317 no. 5839 pp. 787-790
DOI: 10.1126/science.1145220

- REPORT

Ultrafast Flash Thermal Conductance of Molecular Chains

Zhaohui Wang[1,*], Jeffrey A. Carter[1,*], Alexei Lagutchev[1,*], Yee Kan Koh[2], Nak-Hyun Seong[1,*], David G. Cahill[2,3] and Dana D. Dlott[1,3,†]



Breakdown of Fourier's law: experimental confirmation

PRL **101,** 075903 (2008) PHYSICAL REVIEW LETTERS week ending 15 AUGUST 2008

Breakdown of Fourier's Law in Nanotube Thermal Conductors

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(Received 11 March 2008; revised manuscript received 9 July 2008; published 15 August 2008)

We present experimental evidence that the room temperature thermal conductivity (κ) of individual multiwalled carbon and boron-nitride nanotubes does not obey Fourier's empirical law of thermal conduction. Because of isotopic disorder, κ's of carbon nanotubes and boron-nitride nanotubes show different length dependence behavior. Moreover, for these systems we find that Fourier's law is violated even when the phonon mean free path is much shorter than the sample length.

Questions:

- If Fourier's law is not valid, what law should be used instead for 1D crystals to describe heat transfer?
- Can it be derived rationally from the equations of atoms motion?

$$\cancel{h = -\kappa T'} \quad ?$$

Nonsteady heat transfer in 1D harmonic crystal: derivation of the modified Fourier's law

Equations of motion:

$$\ddot{u}_k = \omega_0^2 \left(u_{k-1} - 2u_k + u_{k+1}\right), \qquad \omega_0 = \sqrt{C/m},$$

where u_k is the displacement, m is the particle mass, C is the bond stiffness.

Initial conditions:

$$u_k\big|_{t=0} = 0, \qquad \dot{u}_k\big|_{t=0} = \sigma(x)\rho_k,$$

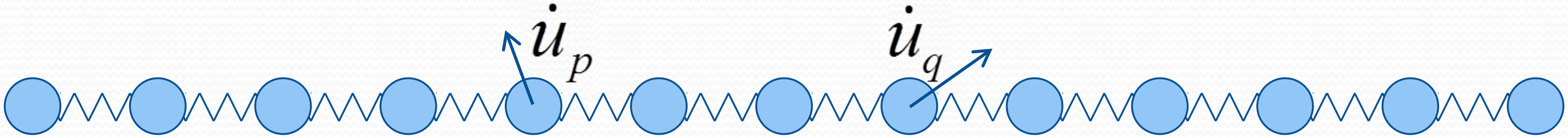
ϱ_k are independent random variables with zero expectation and unit variance;

σ is variance of the initial particle velocity.

The variance is a slowly changing function of the spatial coordinate $x = ka$, where a is the initial distance between neighboring particles.

A.M. Krivtsov, 2015, ArXiv:1509.02506

Nonlocal temperature



$$k_B \theta_{pq} \overset{\text{def}}{=} m \langle \dot{u}_p \dot{u}_q \rangle$$

k_B — the Boltzmann constant, $\langle \ldots \rangle$ — averaging opperator

$$\theta_{pq} = \theta_n(x), \qquad n = q - p, \qquad x = (p+q)/(2a),$$

Initial problem for nonlocal temperature:

$$\ddot{\theta}_n = \frac{1}{4} c^2 (\theta_{n-1} + 2\theta_n + \theta_{n+1})'', \quad \theta_n \big|_{t=0} = \frac{m\sigma^2(x)}{2k_B} \delta_n, \quad \dot{\theta}_n \big|_{t=0} = 0,$$

$c = \omega_0 a$ — sound speed, $\delta_n = 1$ for $n = 0$ and $\delta_n = 0$ otherwise.

Kinetic temperature

Initial problem for nonlocal temperature:

$$\ddot{\theta}_n = \frac{1}{4} c^2 \left(\theta_{n-1} + 2\theta_n + \theta_{n+1}\right)'', \quad \theta_n\big|_{t=0} = \frac{m\sigma^2(x)}{2k_B}\delta_n, \quad \dot{\theta}_n\big|_{t=0} = 0.$$

Relation between kinetic and nonlocal temperature:

$$T(t,x) \overset{\text{def}}{=} m\left\langle \dot{u}_k^2 \right\rangle / k_B = \theta_0(t,x).$$

Initial problem for kinetic temperature:

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \qquad T\big|_{t=0} = T_0(x), \qquad \dot{T}\big|_{t=0} = 0,$$

$c = \omega_0 a$ — sound speed, $m\sigma^2(x)/(2k_B)$ — initial temperature.

A.M. Krivtsov, 2015, ArXiv:1509.02506

Kinetic temperature

Initial problem for kinetic temperature:

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \qquad T\big|_{t=0} = T_0(x), \qquad \dot{T}\big|_{t=0} = 0,$$

Initial problem solution:

$$T(t,x) = \frac{1}{\pi}\int_{-t}^{t} \frac{T_0(x - c\tau)}{\sqrt{t^2 - \tau^2}}\,d\tau,$$

Heat equations comparison

- Classic (Fourier): $$\dot{T} = \beta T''$$
- Hyperbolic (Maxwell-Cattaneo) $$\ddot{T} + \frac{1}{\tau}\dot{T} = \frac{\beta}{\tau} T''$$
- Modified (Krivtsov) $$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T''$$

β — thermal diffusivity, τ — relaxation time, c — sound speed.

Heat conduction laws comparison

- Classic (Fourier): $$h = -\kappa T'$$
- Hyperbolic (Maxwell-Cattaneo) $$\dot{h} + \frac{1}{\tau} h = -\frac{\kappa}{\tau} T'$$
- Modified (Krivtsov) $$\dot{h} + \frac{1}{t} h = -k\rho c^2 T'$$

κ — thermal conductivity, τ — relaxation time,
k — Boltzmann's constant, ρ — density, c — sound speed.

Example 1: sinusoidal temperature disturbance

$$T_0(x) = A \sin \kappa x + B.$$

Solution:

- Temperature: $$T(t, x) = A J_0(\kappa c t) \sin \kappa x + B$$

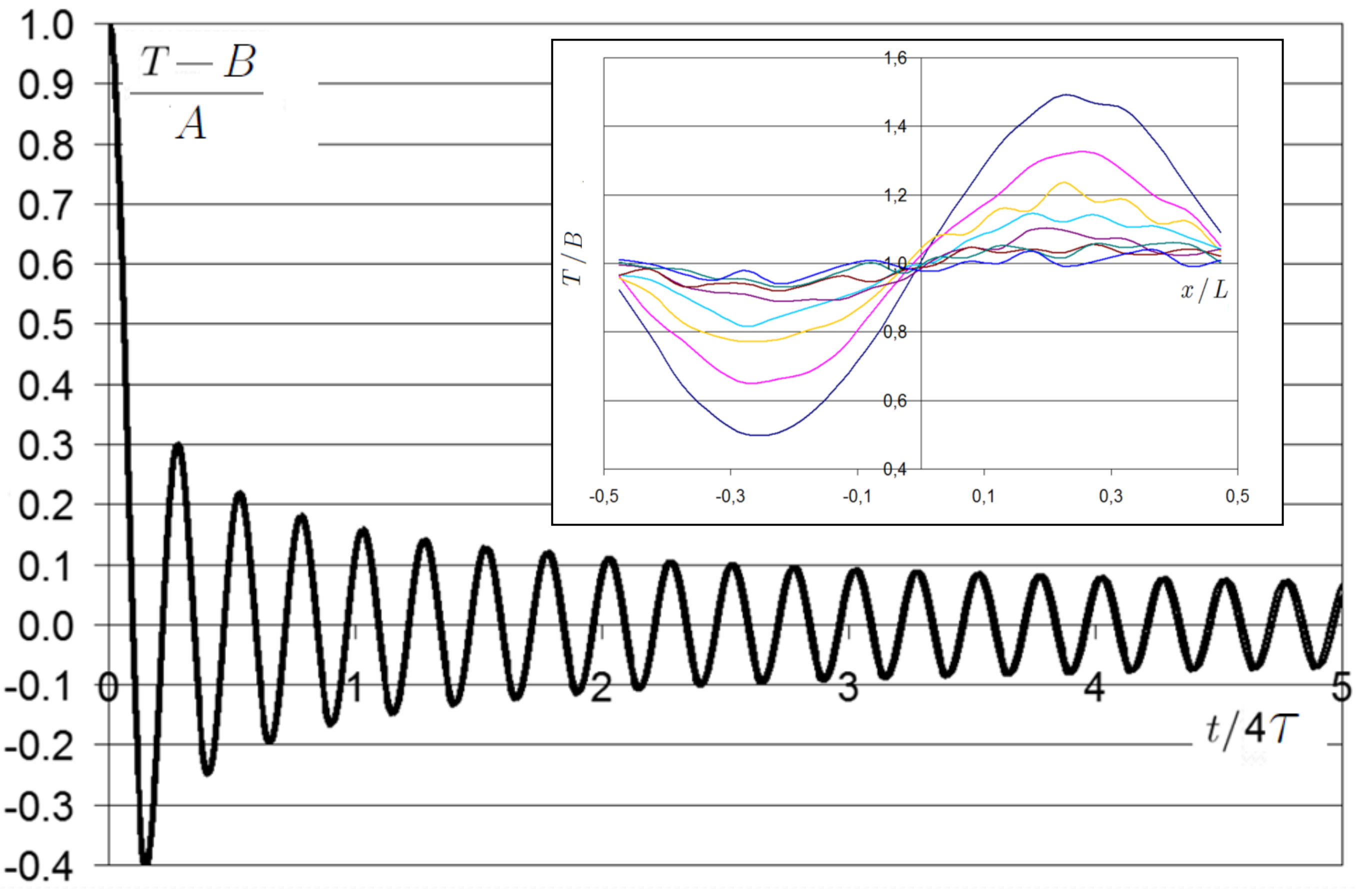
- Heat flux: $$h(t, x) = -k\rho c A J_1(\kappa c t) \cos \kappa x$$

J_0, J_1 — Bessel functions.

k — Boltzmann's constant, ρ — density, c — sound speed.

Decay of the sinusoidal temperature disturbance

$$T(t,x) = AJ_0(\kappa ct)\sin\kappa x + B$$



Example 2: Heat transfer from hot half-space to cold half-space

$T_0(x) = A$ for $x < 0$ and $T_0(x) = 0$ otherwise.

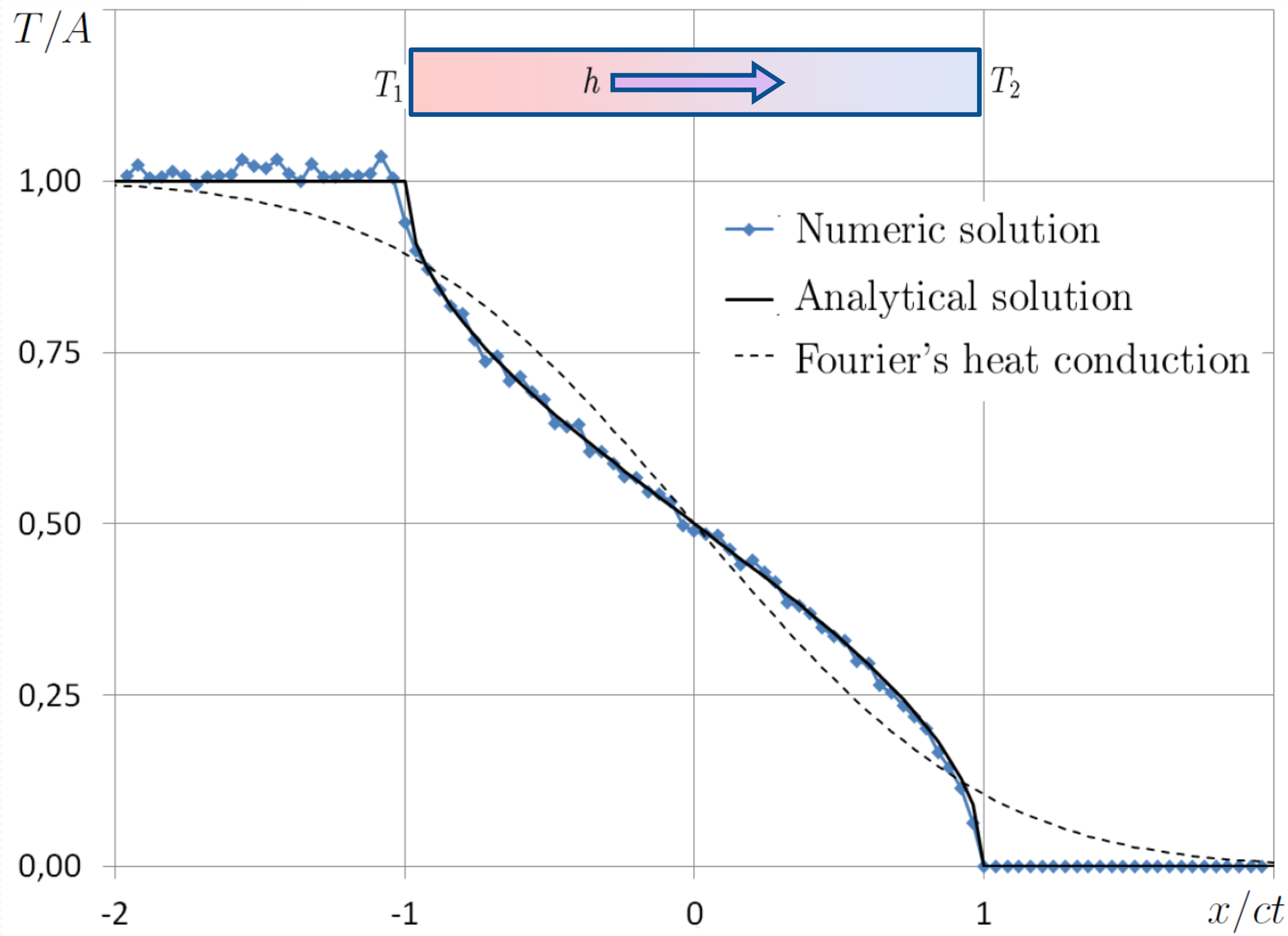
Solution for: $|x| \leq ct$

- Temperature: $$T(t, x) = \frac{A}{\pi} \arccos \frac{x}{ct}$$
- Heat flux: $$h(t, x) = \frac{k\rho A}{\pi t} \sqrt{c^2 t^2 - x^2}$$

k — Boltzmann's constant, ρ — density, c — sound speed.

Heat transfer from “hot” to “cold”

$$T(t,x) = \frac{A}{\pi} \arccos \frac{x}{ct}$$



Conclusions

- Stochastic problems for simple discrete media can be reduced to deterministic problems for generalized discrete media.
- The presented methods allow solving nonstationary problems, where notion of thermodynamic equilibrium is not valid.
- Heat transfer in 1D harmonic crystals is described by the following equations:

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \qquad \dot{h} + \frac{1}{t}h = -k\rho c^2 T'$$

- Ultrafast heat transfer and negligible thermal resistance indicate thermal superconductivity in one-dimensional crystals.

Publications

- A.M. Krivtsov. **On unsteady heat conduction in a harmonic crystal.** 2015, ArXiv:1509.02506.

- A.M. Krivtsov. **Energy Oscillations in a One-Dimensional Crystal.** *Doklady Physics*, 2014, Vol. 59, No. 9, pp. 427–430 (*Доклады Академии Наук*. 2014, том 458, № 3, 279–281.)

Thank you!